A Comparison of Navier Stokes and Network Models To Predict Chemical Transport In Municipal Water Distribution Systems.

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Abstract

We investigate the accuracy of chemical transport in network models for small geometric configurations. Network model have successfully simulated the general operations of large water distribution systems. However, some of the simplifying assumptions associated with the implementation may cause inaccuracies if chemicals need to be carefully characterized at a high level of detail. In particular, we are interested in precise transport behavior so that inversion and control problems can be applied to water distribution networks. As an initial phase, Navier Stokes combined with a convection-diffusion formulation was used to characterize the mixing behavior at a pipe intersection in two dimensions. Our numerical models predict only on the order of 12-14 % of the chemical to be mixed with the other inlet pipe. Laboratory results show similar behavior and suggest that even if our numerical model is able to resolve turbulence, it may not improve the mixing behavior. This conclusion may not be appropriate however for other sets of operating conditions, and therefore we have started to develop a 3D implementation. Preliminary results for duct geometry are presented.

Introduction

In this paper, we investigate the accuracy of chemical transport within water distribution system network models by applying high-fidelity computations to model individual network components. Network models have been used for years to simulate chemical transport within water distribution systems in order to better manage chlorine distribution and water quality. Tools such as EPANET have been developed to efficiently predict hydraulic flow and chemical transport behavior within a system. Due to the extreme size and detail of real-world datasets, simplifying assumptions must be applied to fluid flow and chemical transport in order to reduce computational demands. However, these simplifications often reduce the accuracy of a network model since the impact of small-scale phenomenon is neglected. We believe that the resolution of such small-scale phenomenon is necessary in order to more accurately characterize and remediate a water distribution system during a contamination event.

This work is motivated by the need to utilize novel mathematical algorithms within numerical simulation to support water distribution system management during a contamination event. Our goal is to improve the mitigation performance by leveraging high-fidelity modeling to more accurately characterize the transport of contaminants during an

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event. In response to this need, Laird et al. [9] have developed inversion algorithms to reconstruct a contamination event assuming that measurements of contaminant concentrations are available at sparsely located sensors, and Berry et al. [1] have developed combinatorial methods to provide optimal sensor placement strategies. Although these algorithms have been numerically verified, their utility is limited by the accuracy of the numerical models used to predict or characterize chemical transport.

High-fidelity computational fluid dynamics (CFD) tools have advanced significantly, enabling the characterization of complex phenomena ranging from chemical reactions in chemical vapor depositions [14] to highly turbulent flows using Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) [10,11,12] . Combined with large computational resources, these CFD tools can more accurately characterize fluid flow and chemical mixing in complex geometries. To date, very little work has been performed to characterize the complex, fine-scale chemical transport behavior within the turbulent flows of a water distribution system. For practical purposes, modeling such detail is unnecessary, and perhaps more importantly, too expensive for entire networks. However, the state-of-the-art network model is only as good as the accuracy of its underlying assumptions for the smallest, fundamental physics within these networks. By carefully evaluating the fluid flow behavior at this fundamental level, we hope to extract certain corrections to help improve the accuracy of chemical transport in network models.

During the initial phase of this investigation, we investigate the cross-joint intersection of four pipes (two inflowing, two outflowing). The standard network simulator assumes an even distribution of chemical within the joint based on an instantaneous mixing assumption. Although intuitively we can predict less than perfect mixing under prescribed inlet conditions, it is difficult to quantify the behavior with sufficient accuracy to develop and apply first-order corrections within a network model. We attempt to characterize this mixing behavior assuming no chemical reaction in the system, although chemical reactions can be handled in our current formulation and may be included in the future. The remainder of the paper presents the mathematical formulation for the high fidelity computational fluid dynamics. Numerical and experimental results are presented.

Mathematical Formulation

The final goal of this investigation is to develop a first-order correction for mixing phenomena in network models by more accurately characterizing the chemical transport behavior within important pipe geometries through the use of 3D turbulent Navier-Stokes simulation. To accomplish this goal, we first test smaller components (i.e. pipe joints) in 2D under the assumption of laminar flow or using a Reynolds Averaged Navier-Stokes (RANS) model without resolving the small-scale, unsteady fluctuations of a 3D fully turbulent flow. Eventually, we will build up to a high fidelity characterization consisting of fully-developed 3D turbulence. The underlying physics for these studies is based on the Navier-Stokes equations and convection-diffusion equations. Navier Stokes is based on conservation of mass and momentum. First the conservation of momentum can be formulated as follows:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) - \nabla \mathbf{T} - \rho \mathbf{g} = 0 \quad (1)$$

where ρ is the density, **u** is the velocity vector, t is time, T = -P I + μ is the stress tensor for a Newtonian fluid, P is the hydrodynamic pressure, μ is the viscous stress tensor, and **g** is the gravitational force. Conservation of mass is as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (2)$$

Chemical transport is formulated as a separate convection-diffusion equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\mathbf{u}) - \nabla \cdot (D_{\text{eff}} \nabla C) = 0. \quad (3)$$

where C represents concentration, D_{eff} is the effective diffusion coefficient, and **u** is the velocity field.

Numerical Implementation

The incompressible Navier Stokes equations are solved using MPSalsa [15,16]. Our implementation of incompressible Navier Stokes is designed to handle large datasets on massively parallel computers in addition to an efficient implementation for complex dynamics in three dimensions. The code uses a Petrov Galerkin finite element formulation for unstructured meshes and is capable of solving steady state and transient problems using a fully implicit time integration. The nonlinear systems are solved using inexact Newton methods which in turn depend on Krylov based linear solvers. This implementation (MPSalsa) is capable of resolving turbulence using a variety of Reynolds averaged Navier Stokes (RANS) and Large Eddy simulation (LES) based methods and can handle chemical reactions [8].

Using DNS or LES to more accurately evaluate mixing phenomenon within a water distribution network is computationally demanding, even when modeling is focused on small components of the network. To resolve turbulent flow, a high-resolution 3D mesh is necessary to capture the small-scale effects of turbulence, which results in extensive computational processing and memory use. To alleviate these computational demands and establish insight during the initial stages of this investigation, we limited flow and transport to 2D recognizing that turbulence would not be captured properly. For the purposes of the 2D investigation, we employed an 1152 element mesh on 8 to 16 computational processors to simulate the mixing phenomenon within a 2 inch cross joint (see Figure 1).

The first step in modeling cross-joint mixing was to develop 2D flow inside a hypothetical pipe joint within which chemical tracer could be added to assess the amount of mixing at the

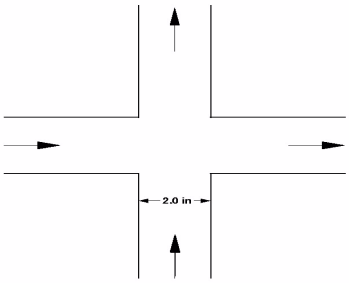

Figure 1 - Schematic of pipe cross-joint type

joint. This flow field was developed by incorporating oscillatory (sinusoidal) boundary conditions at the inlets shown in Figure 1, thereby emulating turbulent-like flow. Inlet bulk velocities were prescribed at 0.78 meters per second, resulting in an average pipe Reynolds number of ~44,000 based on the characteristics of water at 25° C (i.e. viscosity of 8.9 x 10^{-4} kg/m-s, density of 997.0 kg/m^3) and a 2 inch (.0508 meter) pipe diameter. Figure 2 illustrates the velocity field 10 seconds into the 20 second simulation, at which point 32.5 pipe volumes of water have passed through the joint.

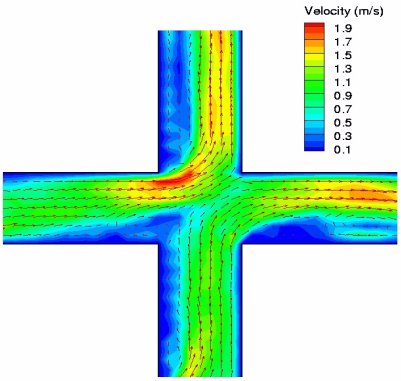

Figure 2 – Velocity field within pipe cross-joint type at 10 seconds simulation time

Although the Reynolds number is well in excess of 2000 suggesting turbulent flow, the 2D model is not capable of fully resolving turbulence, as shown in Figure 2. MPSalsa accounts for subgrid scale turbulent kinetic energy enabling it to compute a turbulent viscosity term(see Figure 3), and therefore is able to predict the general fluid flow characteristics for this geometry.

By definition, this turbulent viscosity represents the turbulent transfer of momentum by eddies. In the case of chemical transport, the term can also be thought of as a coefficient of enhanced diffusion due to mechanical mixing. MPSalsa utilizes the turbulent viscosity to calculate an effective diffusivity D_{eff}

$$D_{\text{eff}} = D_{\text{molecular}} + \frac{\mu_t}{\text{Sc}}, \tag{4}$$

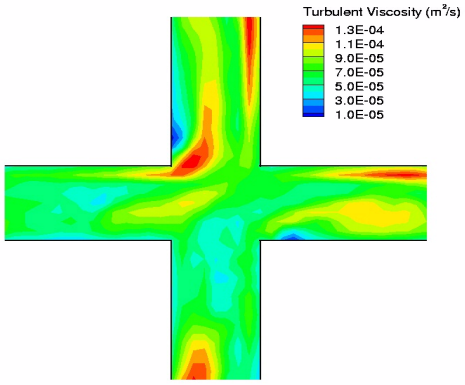

Figure 3 – Turbulent viscosity within pipe cross-joint type at 10 seconds of simulation

where $D_{molecular}$ is the coefficient of molecular diffusion and Sc represents the dimensionless Schmidt number. Therefore, in regions of high turbulent viscosity, one can expect mechanical mixing to dominate the diffusion process. Coupling the velocity field **u** and effective diffusivity above, MPSalsa uses the convection-diffusion equation (3) to simulate chemical transport.

Numerical Results

For this work, cross-joint mixing was simulated by introducing a tracer at the bottom inlet boundary condition while pristine water entered the model from the left inlet (see Figure 1). The degree to which mixing occurred at the cross joint was measured by comparing the outlet flux of tracer at the top and right exit boundaries. Although a direct comparison of the two outlet fluxes is unrealistic (i.e. discrepancies in local pipe velocities most likely result in asynchronous breakthrough), a general trend is observed. Figure 4 illustrates the normalized outlet flux concentrations, averaged across the width of the pipe, over the 20 second simulation.

It is evident that most of the tracer, entering the joint from the bottom inlet, exits to the right following the flow velocity vectors shown in Figure 2. Mixing, defined here as the change

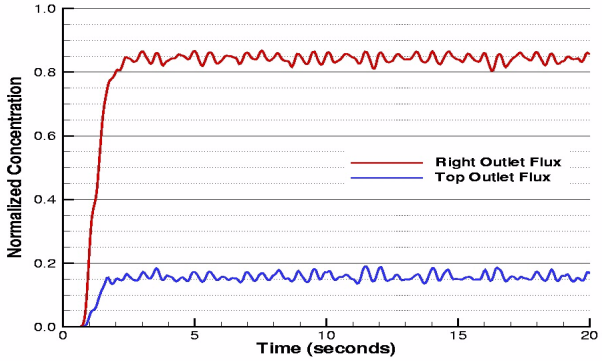

Figure 4 – Normalized simulation tracer breakthrough at outlets

in concentration relative to the inlet tracer concentration

$$\frac{|(C_{\text{in,left}} - C_{\text{out,top}})|}{C_{\text{in, bottom}}} \quad \text{and} \quad \frac{|(C_{\text{in,bottom}} - C_{\text{out,right}})|}{C_{\text{in, bottom}}}, \tag{5}$$

is approximately 13-18% and is clearly not complete as would be the case if both outlet fluxes plotted at 50 %. Figure 5 illustrates snapshots of tracer concentration at 9, 10, and 11 seconds simulation time.

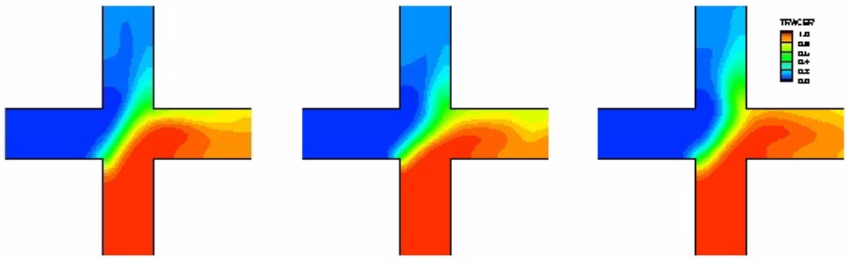

Figure 5 – Tracer concentration within pipe cross-joint type at 9, 10, 11 seconds simulation time

Although flow exceeds a Reynolds number of 2000, the bulk flow clearly interacts in a more laminar manner within the cross joint.

Experimental Verification

In order to verify the results generated by MPSalsa, a physical model of the pipe cross joint above was assembled and experiments were run at approximately the same Reynolds number (i.e. 44,111). This physical model consisted of four 50 gallon tanks interconnected by 2 inch PVC pipe intersecting at a PVC cross joint. Two centrifugal pumps of identical size were placed up-gradient from the cross joint as illustrated in Figure 6. Two tanks, one containing tap water and another containing a NaCl tracer, served as sources for the two pumps which subsequently pumped the water through the joint and into the two outlet tanks.

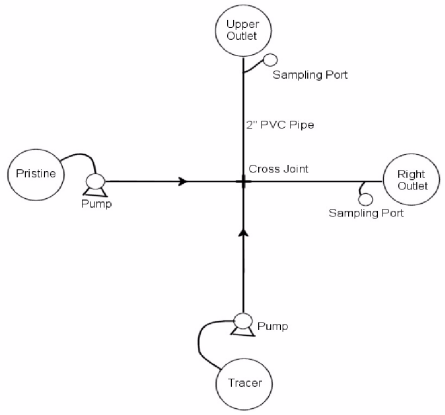

Figure 6 – Schematic of experimental setup

We assumed that the tracer was fully mixed within the bottom inlet tank and within the up-gradient pipes turbulence was fully developed before water passed through the joint. We also assumed that tracer concentration was uniform across the entire pipe cross-section by the time it reached the sampling ports 6 feet down-gradient from the cross joint, which based on mass balance calculations appears to be valid. The experiment ran for 100 seconds, while effluent water was sampled at 10, 25, 40, 55 and 85 seconds. The conductivity of effluent water extracted from the sample ports was compared to that of the tap water (background) and the NaCl mixture (tracer) in the two inlet tanks, and normalized concentrations were calculated. Figure 7 shows the normalized tracer breakthrough at both outlets over time. Based on Equation (5), 12-14% mixing was observed at both outlets. Here, we see that the numerical simulation is close to approximating the experimental results, and since simulated flow within the pipe is more laminar than turbulent, it suggests that turbulence within the numerical model will not increase the mixing in a cross-section significantly. To develop a first order approximation however, numerical simulation can provide an appropriate range of predictions to characterize the behavior of chemicals in other pipe geometries and different operating conditions where turbulence may play a greater role. It is critical therefore to continue to pursue the three dimensional model and try to establish fully resolved turbulence.

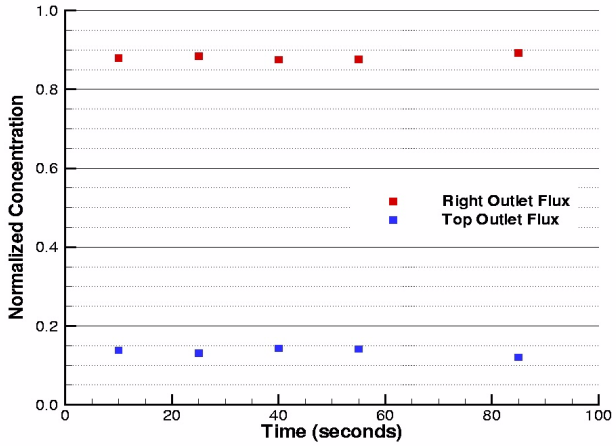

Figure 7 – Normalized experimental tracer breakthrough at outlets.

Ongoing Research - 3D Turbulence Simulation and First Order Corrections

In a closely coordinated but parallel effort, another fluid flow code was utilized to investigate turbulence in 3D. The reasons for selecting another code to investigate turbulence was to 1) efficiently leverage human resources (code familiarity and experience), 2) provide for a verification mechanism (other than limited experimentation), and 3) make use of other capabilities, such as discontinuous Galerkin (DG) methods with the associated advantages of high-order accuracy, local hp-refinement, and multiscale modeling. This code, Sage, uses a new approach to large eddy simulation (LES) that is based on a local variational multiscale (*l*VMS) method [3,4,6] which is an extension of the VMS method of Hughes [2,7] that is extended to support local multiscale modeling on an element-by element basis using DG. Sage has been validated on a variety of laminar flows [5] and the *l*VMS approach within Sage has been carefully studied for planar turbulent channel flows [6,13]. In these studies, *l*VMS is demonstrated not only to be more accurate than the dynamic model for LES but also

simpler to implement, especially on unstructured meshes for complex geometries.

The current work extends our use of *l*VMS to the more complicated cross-section geometry. To date, we have established fully turbulent flow in an inlet section of square duct. Figure 8 shows contours of streamwise momentum on several slices through the computational domain. The results of this single-duct simulation will be used to specify fully-turbulent inflow conditions for the cross-junction model.

Based on the 2D numerical results and laboratory verifications, a first order correction in network models needs to be developed to address chemical transport as a function of geometry, fluid flow dynamics and chemical characterization. Specifically, some obvious parameters can be identified that most likely will provide the foundation for the development of the first order correction scheme, such as 1) Reynolds number, 2) retention time as function of pipe geometry, 3) chemical concentration. To develop a correction strategy, significant numerical studies need to be conducted to quantify the amount of mixing for a range of geometries.

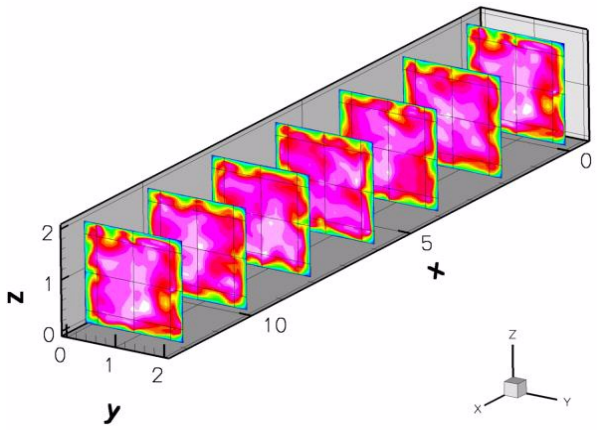

Figure 8 – Fully developed turbulence flow in a duct geometry.

Conclusions

High fidelity numerical and laboratory results indicate that chemical transport behavior is not accurately simulated in the state of the art network models. These network models assume instantaneous mixing and although these network simulators have been successfully used for general operational management, it is not clear that chemical transport can be accurately predicted for contamination events. Contrary to the network model predictions of 50 % in each outlet, our numerical models and laboratory results show 12-14 %. Even though the 2D implementation is not capable of fully resolving turbulence, the numerical model still provides a reasonable match to the laboratory tests, which were conducted in the turbulent regime. This suggests that the small volume at the intersection is not sufficient to allow for complete mixing and that fully developed turbulence in our numerical model may not provide much additional mixing. A three dimensional model has been implemented and we show fully developed turbulence in a simple duct geometry.

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